

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Real or artifactual symmetry breaking in BNB: A fixed-node diffusion Monte Carlo study¹ WISSAM A. AL-SAIDI, CYRUS UMRIGAR, Cornell University — The linear BNB molecule represents one of the most challenging examples of symmetry-breaking effects because of its susceptibility to a second-order Jahn-Teller distortion along the antisymmetric stretching mode. This real symmetry breaking could be confused in calculations with an artifactual one caused by the approximate nature of the theoretical approach. Thus the debate of whether the ground state of BNB is symmetric in the positions of the boron atoms with respect to nitrogen or if this symmetry is broken. Our preliminary investigations with diffusion Monte Carlo shows that the symmetric and the broken symmetry geometries are nearly degenerate, which would suggest a highly floppy quasi-symmetric BNB ground state.

¹Supported by NSF and DOE.

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Date submitted: 04 Dec 2007

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